Submission in Response to NSF CI 2030 Request for Information

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Research Domain, discipline, and sub-discipline

Theoretical and computational atomic and molecular physics and applied mthematics

Title of Submission

Advanced Cyberinfrastructure:The Key Role of the National Science Foundation

Abstract (maximum ~200 words).

As a former Program Director in the Physics Division and Office of Cyberinfrastructure (CI) of the NSF as well as part of a large group who has used and benefited from NSF resources, I felt it would be useful to provide my perspective on where and what the NSF role should be in the evolving national CI.

At NIST, I am responsible for the NIST Digital Library of Mathematical Functions (DLMF). This in an on-line compendium of the properties of the special functions of mathematical physics. The DLMF was conceived in 1997 as a modern successor to the Abromowitz and Stegun (A&S), AMS 55 Handbook of Mathematical Functions, the single most referenced text in the history of NBS/NIST. It contains considerably more information on the special functions than appeared in the original A&S, lots of 3D interactive graphics, far more references to material in the literature and far fewer mathematical tables. It was published in 2010 and involved input from many mathematicians and scientists over the entire globe.
My own research interests are in computational atomic and molecular physics. I develop and apply novel numerical methods to problems involving dynamical processes such as scattering of electrons from atoms and molecules or the interaction of strong electromagnetic with atomic and molecular systems. Many of these problems require large scale computation and the NSF supercomputers and associated people expertise have been invaluable to our work.

Question 1 Research Challenge(s) (maximum ~1200 words): Describe current or emerging science or engineering research challenge(s), providing context in terms of recent research activities and standing questions in the field.

These are reflections of my personal research interests but I suspect the challenges for the future face all computational scientists seeking

quantitative solutions to complex problems in physics and engineering.
During the past decade, it became possible to use advanced CI to provide quantitative solutions to the time evolution of the six-dimensional(two electrons, three coordinates each) Schroedinger equation in the presence of EM fields for He and H2. Much was learned about the effects of electron correlation and how computation can guide and complement experiment in this fast-evolving branch of science. These studies required approximately 10 million cpu hours a year on resources such as Stampede, Comet, SuperMIC and their predecessors. In the future, we would like to study both atoms and in particular molecules having more than two electrons. To date, there have been few studies which have considered the nuclear and well as the electronic degrees of freedom. To go beyond the fixed nucleus approximation is critically important and could easily increase computational requirements by a factor of 10. This will only be possible using an advanced CI that provides not only the computational engines but the people and expertise to use these as the CI evolves in new directions over the next decade.

Question 2 Cyberinfrastructure Needed to Address the Research Challenge(s) (maximum ~1200 words): Describe any limitations or absence of existing cyberinfrastructure, and/or specific technical advancements in cyberinfrastructure (e.g. advanced computing, data infrastructure, software infrastructure, applications, networking, cybersecurity), that must be addressed to accomplish the identified research challenge(s).

This is a complex problem having both obvious and not so obvious elements. The obvious ones are providing a set of resources that can meet the needs of users of advanced CI. When I say advanced CI, I am not restricting my remarks to what are known as power users, important as they may be. There are many scientists that need advanced CI but are not inclined to become experts in ”command line linux” but need to use a CI built by others for scientific advancement. Other users simply cannot get what they need locally and have to turn to the NSF to get their work done. A critical element, which may be less obvious to some, is the need for an advanced CI that is evolving but has enough stability that it is not disruptive to users. There is certainly a tension here since the NSF as THE US open science agency, and very sensitive to the peer review issue, has had difficulty walking this line over the years. I believe there has been progress with the incarnation of the XSEDE progam and other recent developments. These need to continue but I would like to see future developments enlarge the circle of institutions that can participate in these activities and also contribute to the overall US CI. A small step in this direction has been taken to allow universities having resources of their own ”plug into” XSEDE program. This benefits them and also benefits all the users. I would also urge the NSF to keep the management of these larger projects under a single structure while allowing creative, new players to enter and less productive ones to leave. I believe it would be unwise to make a series of individual awards without some coherent management strategy. It would become reminiscent of the days of the centers and the decoherence is not good for the users. To speak a bit more to this point, there has been criticism by some members of the community that the NSF has not really had a well thought out long-range plan for CI. Being a former Program Manager and a user, its clear that there is some truth to this assertion. In other areas such as those in PHY and AST, there are groups such as HEPAP and NSAC which develop a strategic plan for the field which cuts across agencies and sets priorities. This is harder to do in the CI area but it would be nice to see some efforts made to go in that direction. To this end, more coordination with DoE would be nice but again, I am aware of the issues facing the agencies and this is not always possible.

Question 3 Other considerations (maximum ~1200 words, optional): Any other relevant aspects, such as organization, process, learning and workforce development, access, and sustainability, that need to be addressed; or any other issues that NSF should consider.

There are many other considerations to worry about but these can be discussed by others. My main thoughts appear above.